# Machine learning: Part 2

- Unsupervised Learning: $k$-means algorithm
- Learning from incomplete Data: EM algorithm

*Slides based on those of D. Poole and A. Mackworth

# Unsupervised learning

- Unsupervised learning is the problem of identifying multiple categories in a collection of objects.
- The problem is unsupervised because the category labels are not given.
- *e.g.*, classification of stars by astronomers
- In hard clustering, each example is placed definitively in a class.
- In soft clustering, each example has a probability distribution over its class.

# EM Algorithm for clustering

- Start with a random theory or randomly classified data
- Repeat the following two steps:
  - E-step generates the expected classification for each example.
  - M-step generates the best theory using the current classification of data.
- We consider two instances of the EM algorithm

# $k$-means algorithm

Used for hard clustering.

Inputs:

- training examples
- the number of classes, $k$

Outputs:

- a prediction of a value for each feature for each class
- an assignment of examples to classes

# $k$-means algorithm formalized

- $E$ is the set of all examples
- the input features are $X_1, \ldots, X_n$
- $val(e, X_j)$ is the value of feature $X_j$ for example $e$.
- there is a class for each integer $i \in \{1, \ldots, k\}$.

The $k$-means algorithm outputs

- a function $class : E \rightarrow \{1, \ldots, k\}$.
  $class(e) = i$ means $e$ is in class $i$.
- a $pval$ function where $pval(i, X_j)$ is the prediction for each example in class $i$ for feature $X_j$.

# $k$-means algorithm formalized

The sum-of-squares error for $class$ and $pval$ is

$$\sum_{e \in E} \sum_{j=1}^{n} \left(pval(class(e), X_j) - val(e, X_j)\right)^2 .$$

Aim: find $class$ and $pval$ that minimize sum-of-squares error.

Initially, randomly assign the examples to the classes.
Repeat the following two steps:

- For each class $i$ and feature $X_j$,

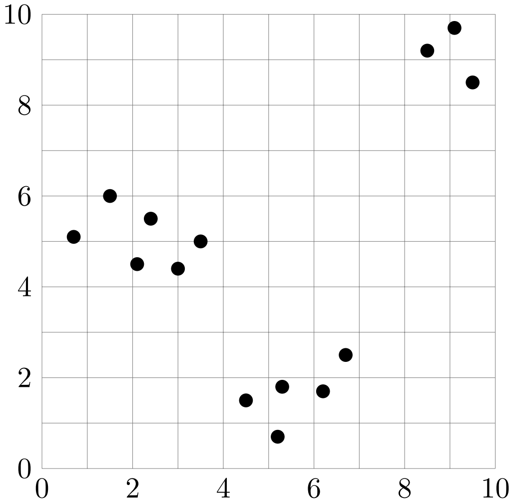
$$pval(i, X_j) \leftarrow \frac{\sum_{e:class(e)=i} val(e, X_j)}{|\{e : class(e) = i\}|},$$

- For each example $e$, assign $e$ to the class $i$ that minimizes

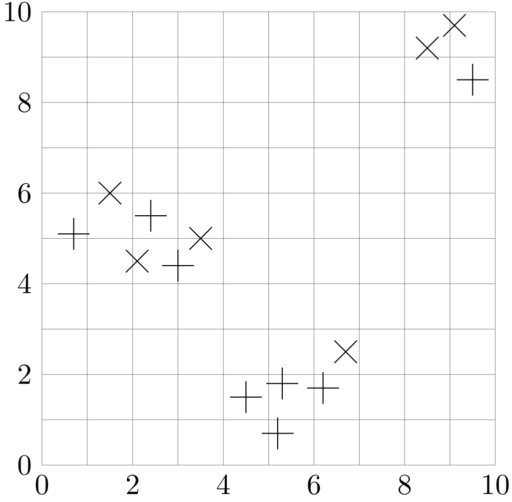
$$\sum_{j=1}^{n} (pval(i, X_j) - val(e, X_j))^2 .$$

until the second step does not change the assignment of any example.

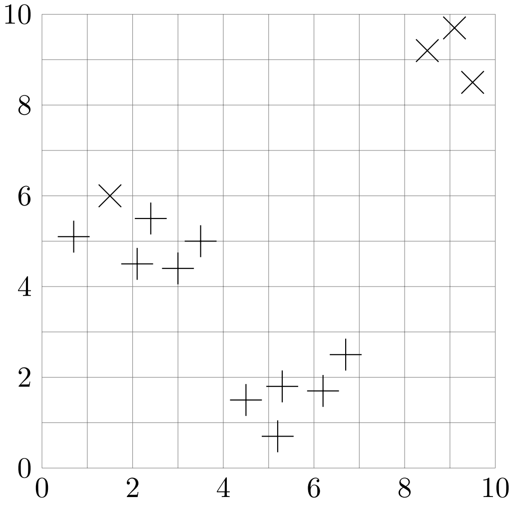
# Example Data



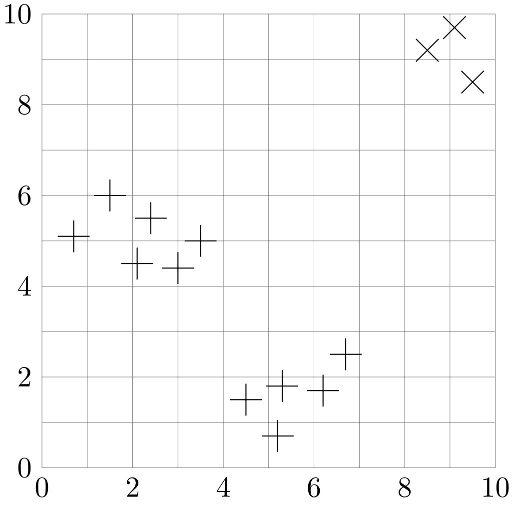
# Random Assignment to Classes



# Assign Each Example to Closest Mean



# Ressign Each Example to Closest Mean




Stable assignment found

# Other clustering results

- A different initial assignment can give different clustering.
- One clustering is for the lower points to be in one class, and for the other points to be in another class.
- Running the algorithm with three classes would separate the data into the top-right, the left-center, and the lower clusters.

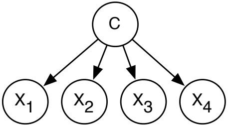
# Properties of $k$-means

- This algorithm will eventually converge to a local minimum.
- It is not guaranteed to converge to a global minimum.
- Increasing $k$ can always decrease error until $k$ is the number of different examples.

# EM algorithm

- Used for soft clustering — examples are probabilistically in classes.
- $k$-valued random variable $C$

Model




Data

| $X_1$ | $X_2$ | $X_3$ | $X_4$ |
|---|---|---|---|
| $t$ | $f$ | $t$ | $t$ |
| $f$ | $t$ | $t$ | $f$ |
| $f$ | $f$ | $t$ | $t$ |
| | ... | | |

➪ Probabilities

$P(C)$
$P(X_1|C)$
$P(X_2|C)$
$P(X_3|C)$
$P(X_4|C)$

# EM Algorithm Overview

- Repeat the following two steps:
  - E-step give the expected number of data points for the unobserved variables based on the given probability distribution.
  - M-step infer the (maximum likelihood or maximum aposteriori probability) probabilities from the data.
- Start either with made-up data or made-up probabilities.
- EM will converge to a local maxima.

# EM algorithm

统计

M-step

| $X_1$ | $X_2$ | $X_3$ | $X_4$ | $C$ | *count* |
|---|---|---|---|---|---|
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| $t$ | $f$ | $t$ | $t$ | $1$ | $0.4$ |
| $t$ | $f$ | $t$ | $t$ | $2$ | $0.1$ |
| $t$ | $f$ | $t$ | $t$ | $3$ | $0.5$ |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |

$P(C)$
$P(X_1|C)$
$P(X_2|C)$
$P(X_3|C)$
$P(X_4|C)$

E-step

贝叶斯

得到P（C|Xi），计算每个样例对应各个C的可能性，再正则化

# Augmented data – E step

Suppose $k = 3$, and $dom(C) = \{1, 2, 3\}$.
$P(C = 1 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.407$
$P(C = 2 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.121$
$P(C = 3 | X_1 = t, X_2 = f, X_3 = t, X_4 = t) = 0.472$:

| $X_1$ | $X_2$ | $X_3$ | $X_4$ | $Count$ |
|---|---|---|---|---|
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $t$ | $f$ | $t$ | $t$ | 100 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |

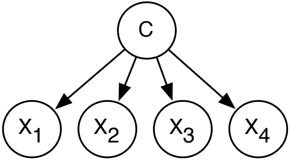
$\longrightarrow$

$A[X_1, \ldots, X_4, C]$

| $X_1$ | $X_2$ | $X_3$ | $X_4$ | $C$ | $Count$ |
|---|---|---|---|---|---|
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
| $t$ | $f$ | $t$ | $t$ | 1 | 40.7 |
| $t$ | $f$ | $t$ | $t$ | 2 | 12.1 |
| $t$ | $f$ | $t$ | $t$ | 3 | 47.2 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |

# M step

| $X_1$ | $X_2$ | $X_3$ | $X_4$ | $C$ | $Count$ |
|---|---|---|---|---|---|
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| $t$ | $f$ | $t$ | $t$ | 1 | 40.7 |
| $t$ | $f$ | $t$ | $t$ | 2 | 12.1 |
| $t$ | $f$ | $t$ | $t$ | 3 | 47.2 |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |



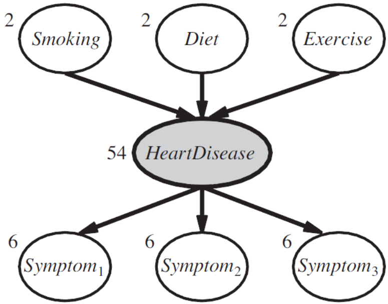

统计

$$P(C{=}v_i) = \frac{\sum_{t \models C=v_i} Count(t)}{\sum_t Count(t)}$$

$$P(X_k = v_j | C{=}v_i) = \frac{\sum_{t \models C=v_i \wedge X_k=v_j} Count(t)}{\sum_{t \models C=v_i} Count(t)}$$

# Learning with hidden variables

- Many real-world problems have hidden (a.k.a latent) variables

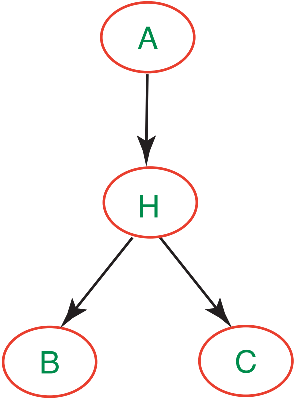



A simple diagnostic network for heart disease

- Hidden variables complicate the learning problem.

# EM algorithm

- Repeat the following two steps:
  - E-step give the expected number of data points for the unobserved variables based on the given probability distribution. Requires probabilistic inference.
  - M-step infer the (maximum likelihood) probabilities from the data. This is the same as the fully observable case.
- Start either with made-up data or made-up probabilities.
- EM will converge to a local maxima.




- What if we had only observed values for $A$, $B$, $C$?

| $A$ | $B$ | $C$ |
|---|---|---|
| $t$ | $f$ | $t$ |
| $f$ | $t$ | $t$ |
| $t$ | $t$ | $f$ |
| | $\dots$ | |

# EM algorithm

Augmented Data

| $A$ | $B$ | $C$ | $H$ | $Count$ |
|---|---|---|---|---|
| $t$ | $f$ | $t$ | $t$ | 0.7 |
| $t$ | $f$ | $t$ | $f$ | 0.3 |
| $f$ | $t$ | $t$ | $f$ | 0.9 |
| $f$ | $t$ | $t$ | $t$ | 0.1 |
| | $\cdots$ | | | $\cdots$ |

E-step

M-step

Probabilities

$P(A)$
$P(H|A)$
$P(B|H)$
$P(C|H)$